Lawrence Livermore National Laboratory

Science & Technology

January/February 2011

Imaging Molecules in Motion

Also in this issue:

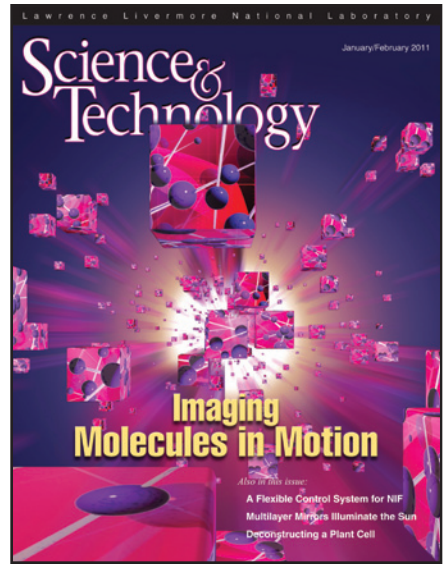
A Flexible Control System for NIF

Multilayer Mirrors Illuminate the Sun

Deconstructing a Plant Cell

About the Cover

The Linac Coherent Light Source (LCLS) produces ultrashort x-ray pulses and is designed to enable scientists to take stop-action pictures of atoms and molecules in motion before the powerful beam destroys the sample. Located at the Department of Energy's SLAC National Accelerator Laboratory in Menlo Park, California, the LCLS project is a collaboration of SLAC; Lawrence Livermore, Argonne, Brookhaven, and Los Alamos national laboratories; and the University of California at Los Angeles. As described in the article beginning on p. 4, Livermore researchers were among the first to conduct experiments at LCLS.



Cover design: Amy E. Henke; illustration: Kwei-Yu Chu

About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

The Laboratory is operated by Lawrence Livermore National Security, LLC (LLNS), for the Department of Energy's National Nuclear Security Administration. LLNS is a partnership involving Bechtel National, University of California, Babcock & Wilcox, Washington Division of URS Corporation, and Battelle in affiliation with Texas A&M University. More information about LLNS is available online at www.llnsllc.com.

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the Web at str.llnl.gov.

National Nuclear Security Administration

Prepared by LLNL under contract
DE-AC52-07NA27344

Science & Technology Review

January/February 2011

Lawrence
Livermore
National
Laboratory

Contents

Feature

Research Highlights

Departments

S&TR Staff

Scientific Editor
Kerri J. M. Blobaum

Managing Editor
Ray Marazzi

Publication Editor
Pamela MacGregor

Writers
Arnie Heller, Rose Hansen, and Caryn Meissner

Art Director
Amy E. Henke

Designers
Brian Chavez and Amy E. Henke

Proofreader
Carolin Middleton

Print Coordinator
Charlie M. Arteago, Jr.

S&TR, a Director's Office publication, is produced by the Technical Information Department under the direction of the Office of Planning and Special Studies.

S&TR is available on the Web at str.llnl.gov

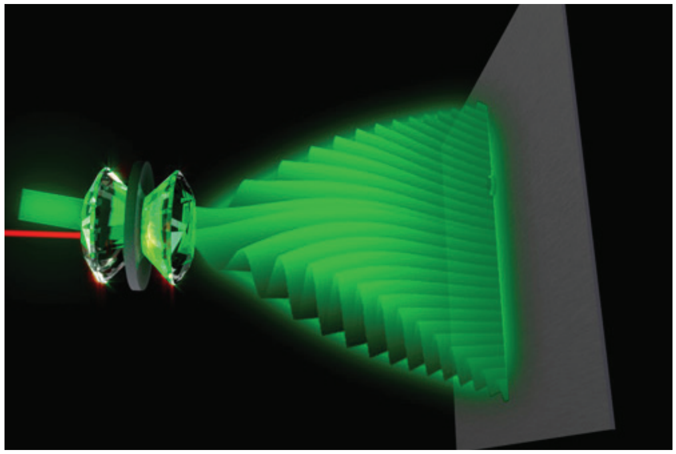
Printed in the United States of America

Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

UCRL-TR-52000-11-1/2
Distribution Category UC-99
January/February 2011

Sound Measure in Materials

A team of Laboratory scientists has developed an adaptable and precise technique to measure the speed of sound in materials and help improve large-scale explosives testing. The new technique is more versatile and easier to use compared to two primary conventional techniques that are technically challenging and require relatively high-fluence beams or pulses, which can induce photoreactions or physically alter sample properties.



In the experiments, a variation of the photoacoustic effect was introduced and applied to highly photosensitive metaboric acid encapsulated in a high-temperature diamond anvil cell (at right). This new variation of photoacoustic light scattering offers several technical advantages over conventional methods. For example, between 10 and 10,000 times less fluence (laser-light power per unit time) is required to measure sound velocity. In this method, a metal strip absorbs a short pulse of laser light and then functions as a transducer to launch a broadband pulse into the surrounding medium. When a second optical pulse strikes the transducer, the transducer passively generates a signal. Speeds of sound can then be measured downstream from the sample container.

Data acquired enabled the first-ever semi-empirical predictions of boron-containing explosive reactions. These results have implications for geodynamic, geochemical, and shock-induced processes, which are often limited by the lack of knowledge of high-pressure equations of state for relevant fluids. The team's findings appeared in the September 21, 2010, online edition of the *Journal of Physical Chemistry Letters*.

Contact: Joseph Zaug (925) 423-4428 (zaug1@llnl.gov).

Understanding Beta Cell Replication

Lawrence Livermore scientist Bruce Buchholz, with collaborators from the National Institutes of Health, used the Laboratory's Center for Accelerator Mass Spectrometry to measure the amount of carbon-14 in DNA in beta cells, which make insulin in the human body, and found that after age 30 the body does not create any new beta cells. The question of whether beta cells replicate after birth has remained an open issue, one that is critically important for designing therapies for diabetes.

Carbon-14 atmospheric concentration levels remained relatively stable until the Cold War, when aboveground nuclear tests caused a sharp increase. This spike in atmospheric carbon-14, which has decreased slowly since the end of aboveground testing in 1963, serves as a chronometer of the past 57 years. Because DNA is stable after a cell has gone through its last cell division, the concentration of carbon-14 in DNA serves as a date marker for when a cell was born and can be used to date cells in humans. "We found that beta cells turn over up to about age 30, and there they remain throughout life," says Buchholz. "The findings have implications for both type 1 and type 2 diabetes."

Research is currently being done in stem cell therapies to replace lost beta cells for both types of diabetes. "But with these new findings, it isn't clear how easy it will be to get the body to make more beta cells in adulthood, when it is not a natural process," says Buchholz. The research appeared in the October 2010 issue of *The Journal of Clinical Endocrinology and Metabolism*.

Contact: Bruce Buchholz (925) 422-1739 (buchholz2@llnl.gov).

Bonding and Stability in Transition Metals

A team of scientists has explored why the group-VB transition metals (vanadium, niobium, and tantalum) can change crystal structure (phase) when they are compressed and alloyed with small amounts of a neighboring metal. The team's results, published in the October 20, 2010, edition of *Physical Review B*, undermine the conventional thought that these metals only solidify with highly symmetric atomic arrangements in cubic and hexagonal cells. Livermore's Alexander Landa and Per Söderlind, along with colleagues from the University of Pittsburgh, Hewlett-Packard, the Royal Institute of Technology in Sweden, the University of Hamburg in Germany, and Uppsala University in Sweden, discovered highly unusual phases with atoms found in rhombohedral symmetry, where the cells are distorted with non-90-degree angles.

The research builds on an earlier study showing that electronic structure combined with electrostatic energies can lead to destabilization of the normal body-centered-cubic phase when these metals are compressed or alloyed. In addition to clarifying the fundamental physics of chemical bonding in these common metals, the results give insight into mechanical properties such as strength.

Contact: Alexander Landa (925) 424-3523 (landa1@llnl.gov) or Per Söderlind (925) 423-4667 (soderlind1@llnl.gov).

World's Most Intense X-Ray Laser Focuses on Livermore Science

THE Linac Coherent Light Source, or LCLS, is the brightest x-ray source in the world and the first x-ray laser available for use by scientists worldwide. It is also the most significant scientific facility built to date in the new millennium by the Department of Energy's Office of Science.

As described in the article beginning on p. 4, Livermore scientists are leaders in applying this unique instrument. Using its unprecedented spatial and temporal resolution, they are studying the most fundamental processes that occur in materials and for the first time are capturing atoms and molecules in motion. The Laboratory has been interested in developing x-ray lasers for several decades. In 1984, scientists demonstrated the world's first laboratory x-ray laser on Livermore's two-beam Novette laser, and in 1996, they built the tabletop COMET x-ray laser at the Laboratory's Jupiter Laser Facility.

Livermore has been closely involved with LCLS since its conception. Our involvement began with an experiment at Brookhaven National Laboratory called VISA, which in 2001 demonstrated the feasibility of a process called self-amplified spontaneous emission (SASE), the basis of LCLS's extraordinarily bright and coherent x-ray pulses. The experiment's success contributed to the decision by the Energy Department to build the $420 million LCLS at the SLAC National Accelerator Laboratory in Menlo Park, California.

During the LCLS research and development phase, Livermore invested Laboratory Directed Research and Development funds toward showing that x-ray optics could be built to withstand the intense x-ray fluences LCLS would generate. During construction, we partnered with SLAC and Argonne National Laboratory to complete the project on time and within budget. Following the facility's commissioning, Livermore researchers began an experimental program to explore the behavior of materials under extreme conditions of temperature and pressure. Our researchers have been among the most successful competitors for beam time on LCLS and have led and collaborated on a number of pioneering experiments conducted with partners from universities and research centers in the U.S. and Europe.

Our experimental program focuses on three broad categories. First, we are advancing the field of x-ray quantum electronics. Experiments led by Nina Rohringer are demonstrating the ability of the main LCLS beam to "pump" a secondary x-ray beam of greater coherence using a gaseous target. Second, in experiments led by Stefan Hau-Riege, we are advancing materials science by studying the damage caused by intense x-ray pulses. Finally, we are imaging biomolecules such as proteins and viruses. These experiments, led by Henry Chapman of the University of Hamburg (formerly of Livermore) and Matthias Frank, are developing the methods for precise injection of biomolecules. The work is a step toward unraveling the structure and operation of membrane proteins that control the cellular exchange of chemicals with the environment. Successful imaging will benefit fields ranging from human health to bioenergy.

The ability of LCLS to examine the physical processes in materials under extreme conditions is directly relevant to the Laboratory's national security mission, in particular its stockpile stewardship responsibilities, where understanding the response of materials to high pressures and temperatures is critical to predicting how nuclear explosives function. LCLS also offers a complementary capability to experiments conducted on the National Ignition Facility, the world's most energetic laser and the center of Livermore's high-energy-density research.

Lessons learned at LCLS will benefit x-ray lasers now being planned in Europe and Japan. LCLS is the second large facility using SASE. The first was the free-electron laser FLASH developed at the Deutsches Elektronen-Synchrotron in Hamburg, Germany, which generates extreme ultraviolet photons. Many Livermore experiments being conducted on LCLS were first demonstrated on FLASH, which is scheduled for an upgrade to an x-ray laser source similar to LCLS. Working on this new generation of x-ray sources, Laboratory scientists will continue to push the frontiers of science and enhance our nuclear security.

■ William H. Goldstein is associate director for Physical and Life Sciences.

GROUNDBREAKING SCIENCE

Experiments at the Linac Coherent Light Source aim to advance the understanding of chemistry, physics, materials science, and life itself.

In fall 2009, researchers conducted the first experiments at the Linac Coherent Light Source (LCLS). Shown here is the Undulator Hall. (Courtesy of SLAC National Accelerator Laboratory.)

with the WORLD'S BRIGHTEST X RAYS

LIVERMORE researchers have been among the first to use the Linac Coherent Light Source (LCLS), which produces ultrashort x-ray pulses more than a billion times brighter than ever produced on Earth. Located at the Department of Energy's SLAC National Accelerator Laboratory in Menlo Park, California, LCLS is designed to enable scientists to take stop-action pictures of atoms and molecules in motion, shedding light on the fundamental processes of chemistry, physics, materials science, electronics, medicine, and life itself.

The LCLS project is a collaboration of SLAC; Lawrence Livermore, Argonne, Brookhaven, and Los Alamos national laboratories; and the University of California (UC) at Los Angeles. Livermore experts designed and fabricated the optics that transport the x-ray beam to chambers in two experimental halls. These mirrors help control the size and direction of the x-ray beam. Additional detectors fabricated by Livermore help diagnose x-ray beam properties such as intensity.

Groundbreaking for the $420 million facility took place in October 2006. At the dedication ceremony August 16, 2009, SLAC Director Persis Drell said, "For some disciplines, this tool will be as important to the future as the microscope has been to the past." Livermore scientists helped to characterize and troubleshoot the x-ray pulses in preparation for initial experiments in October 2009. They also led or contributed to several international collaborations that conducted some of the first scientific experiments on LCLS.

LCLS uses the linear accelerator (linac) at SLAC National Accelerator Laboratory to create x rays of unparalleled brightness and extremely short duration. (Courtesy of SLAC National Accelerator Laboratory.)

Light Source Shines

LCLS is the world's most powerful x-ray free-electron laser (XFEL), producing pulses that are much brighter than those generated at any other x-ray laser facility (up to 10^{12} photons per fleeting pulse). (See the box on p. 7.) While traditional optical lasers generate light from excited atoms, FELs use unattached, or "free," electrons moving through a vacuum chamber at nearly the speed of light to create their beams. FEL photons are coherent, meaning they act in unison, making them well suited for imaging applications.

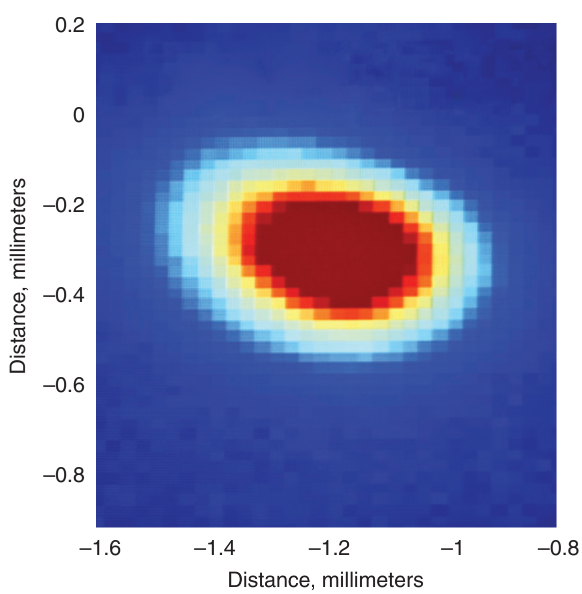
The laser beam's photons have wavelengths of about 0.15 nanometers, about 10 times shorter than can be produced by other XFELs, which produce "soft" or longer wavelength x rays. A tenth of a nanometer (the diameter of a hydrogen atom) is the ideal wavelength for studying atoms and molecules and for providing new information about the atomic-level structure and dynamics of many materials.

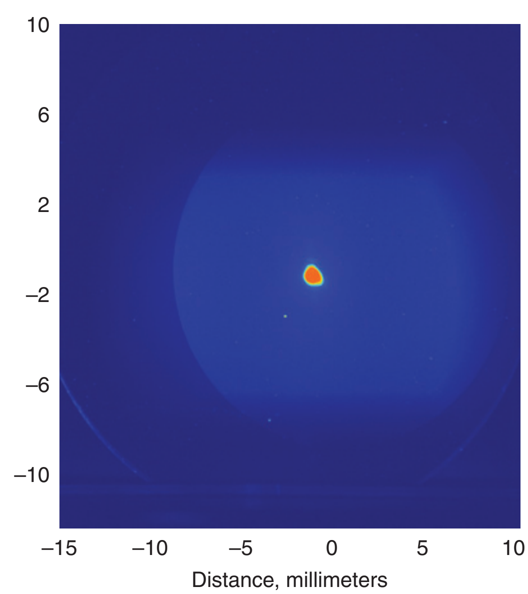
The x-ray laser pulses are of extremely short duration, lasting between a mere 10 and 100 femtoseconds (100 femtoseconds equals 100-quadrillionths of a second) and repeating 120 times per second. To put this extraordinarily short pulse in perspective, consider that light races to the moon in less than 1.3 seconds but travels just the thickness of a sheet of paper in 150 femtoseconds.

Thanks to their brightness, coherence, short wavelength, and extremely brief pulse duration, LCLS x rays will allow scientists to examine atomic-scale objects. Many fundamental processes, such as chemical and biochemical reactions, involve rearrangements of atoms and molecules that occur on timescales of femtoseconds. By sequencing separate stop-action images taken with LCLS pulses, scientists will be able to create time-resolved movies, permitting them to view chemical bonds forming and breaking in real time, such as phase transitions at the atomic level (for example, ice

Livermore scientists designed and built the LCLS x-ray transport optics and diagnostics suite. One of the suite's instruments is the x-ray free-electron laser energy monitor, which won a 2010 R&D 100 Award for being one of the year's most important industrial innovations. (See *S&TR*, October/November 2010, pp. 8–9.)

(right) An image of "first light" at LCLS in April 2009 shows an approximate 0.2-millimeter laser spot, despite having traveled more than 3 kilometers from its source. (far right) An x-ray laser pulse is viewed from the facility's main control center. A point of coherent laser light is surrounded by dimmer noncoherent light. (Courtesy of SLAC National Accelerator Laboratory.)





becoming water). Researchers also expect to create three-dimensional holograms of biomolecules.

In another type of LCLS experiment, some of the x rays scatter when they hit the sample. These deflected x rays strike a detector, and then scientists examine the pattern of diffraction. Although the powerful beam destroys each sample, the ultrashort pulse generates diffraction data before that happens. Livermore researchers have accumulated and integrated thousands of diffraction patterns to develop algorithms for converting the data into usable images.

Collaborators Qualify the Beam

"The facility has been running very well, almost from the start," says physicist Stefan Hau-Riege, who leads one of the Livermore experimental teams. During the summer and fall of 2009, Hau-Riege helped commission the laser. Early experiments achieved an in-depth understanding of how the beam interacts with matter as well as its operating characteristics, including the exposure required to damage materials.

LCLS experiments are performed at one of six end-stations, and the initial experiments were conducted at the atomic, molecular, and optical (AMO) end-station. This end-station, which includes x-ray optics that help focus the beam, is designed to study the effects of soft x rays (wavelengths of 0.6 nanometers and above) on atoms and molecules in gases.

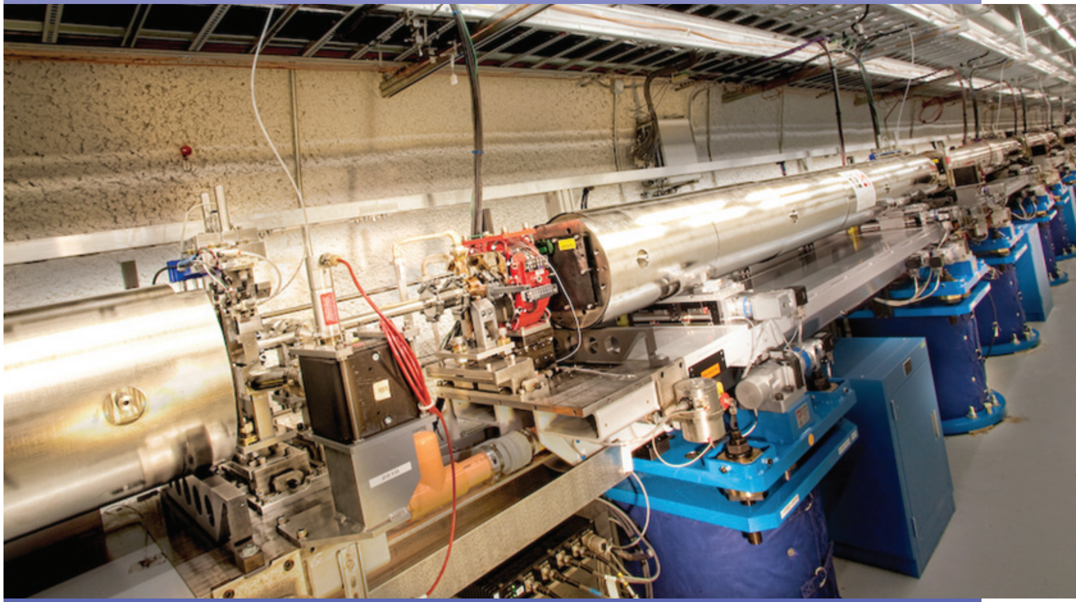
In one experiment, Hau-Riege used a 10-micrometer-diameter x-ray beam to etch the initials LCLS, about 1.5 millimeters wide, into a piece of boron carbide, a superhard substance used in accelerator shielding. (See the figure on p. 8.) To examine how the laser affects solid materials and to determine damage thresholds, the team exposed the boron carbide sample to different beam intensities and wavelengths. By moving the AMO's sample stage in minute increments, the team spelled the laser's initials in small craters blown out of the boron carbide. The

X Rays: A Short Primer

Visible light is only a small part of the electromagnetic spectrum, which also includes radio waves, microwaves, infrared light, ultraviolet light, x rays, and gamma rays. The wavelength of light determines how small a structure we are able to see. For example, the wavelength of visible light is slightly smaller than cells and bacteria, which is why we can see them under a light microscope. Atoms have dimensions on the order of a tenth of a nanometer (a billionth of a meter), so scientists need to use a much shorter wavelength, namely short-wavelength (hard) x rays, for probing atomic structure. As a result, x rays, discovered in 1895 by German physicist Wilhelm Röntgen, have been scientists' principal means of unraveling the positions of atoms in solids from metals to proteins.

The Linac Coherent Light Source (LCLS) is the first machine of its type to probe matter with hard x rays. The facility takes up one-third of the 3-kilometer-long linear accelerator at the SLAC National Accelerator Laboratory. For more than 40 years, SLAC's linear accelerator (or linac) has produced high-energy electrons for physics experiments. Scientists are now using the linac to create x-ray pulses more than a billion times brighter than the most powerful existing sources, the so-called synchrotron sources. Synchrotrons produce streams of x-ray photons with pulses too long to explore the dynamic motion of molecules. Because LCLS can produce pulses of extremely short duration, it can achieve brightnesses significantly higher than synchrotron facilities.

SLAC's linac accelerates very short pulses of electrons to 99.99999 percent the speed of light. LCLS then takes them through a 100-meter-long stretch of alternating magnets in the Undulator Hall that force the electrons to travel back and forth. The process gives off extremely bright x rays with a wavelength of about a ten-billionth of a meter, with each pulse as short as a few quadrillionths of a second. The emitted x rays become synchronized as they interact with the electron pulses, thereby creating the world's brightest x-ray laser pulse. Each 100-femtosecond pulse, produced with a repetition frequency up to 120 hertz (currently 60 hertz), contains more than a trillion (10^{12}) photons with energies from 500 to 10,000 electronvolts.



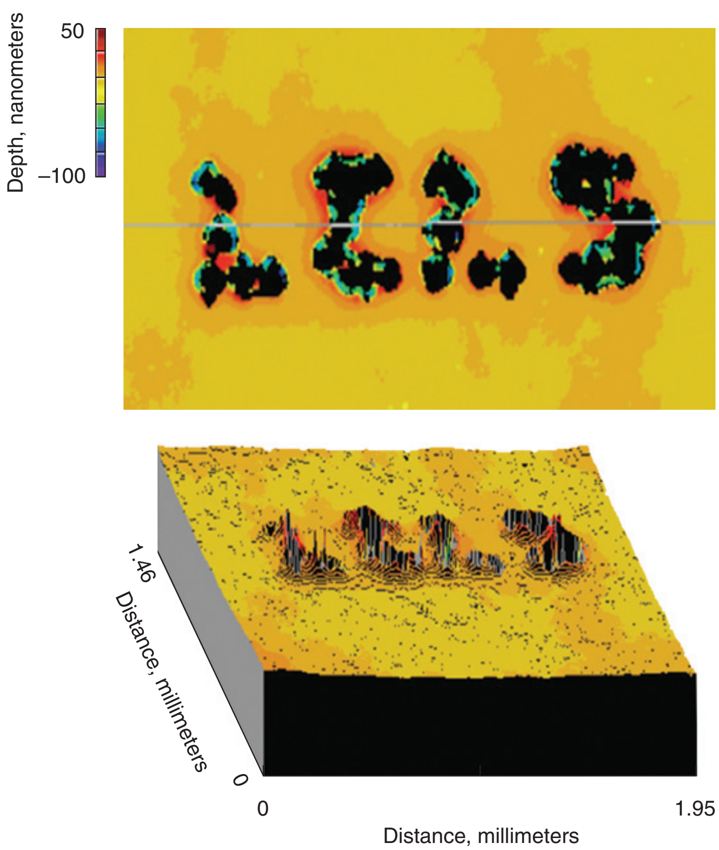
Extremely bright x rays are produced in the Undulator Hall of LCLS. (Courtesy of SLAC National Accelerator Laboratory.)

imprinted initials then served as a baseline for studying the effects of tests at lower x-ray energies.

To assess the depth of the x-ray-induced craters, the team used an interferometer, an instrument that measures the distance light travels as it bounces from the sample to a detector. The researchers further assessed the extent of the damage with scanning electron and atomic force microscopes.

In another experiment, the team used an XFEL energy monitor, one of three installed at LCLS, to study the interaction between nitrogen gas and x-ray pulses with energies up to 8 kiloelectronvolts. The energy monitor, developed by Hau-Riege and Livermore colleagues, measures the pulse-by-pulse energy in real time without being damaged by the beam and with minimal effect on beam quality. The total pulse energy is inferred from x-ray-induced ultraviolet fluorescent light, which is generated by the nitrogen gas and detected by the device's photon-multiplier tubes.

"Understanding how intense x rays interact with atoms and molecules is critical to being able to take the best images and to correctly interpret the diffraction data," says Hau-Riege. The nitrogen gas experiment was performed upstream from the LCLS mirrors, which gave experimenters access to the full range of potential energies. "The sweet spot for conducting atomic-resolution imaging experiments is about 8 kiloelectronvolts," he says. At higher energies, light undergoes Compton scattering, a phenomenon where scattered x rays have different wavelengths than the incident x rays, degrading the diffraction patterns. At lower energies, sample damage is a severe problem because more of the photons are absorbed by the material. Collaborators on the nitrogen experiments included researchers from SLAC and the Deutsches Elektronen-Synchrotron (DESY) in Hamburg, Germany.



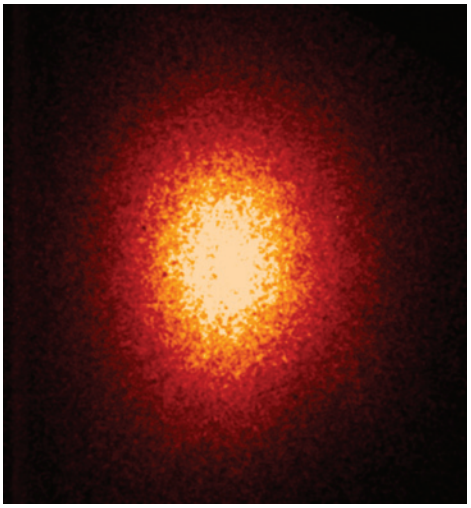
Livermore researchers were among the first to commission LCLS and determine the beam exposure required to damage materials. (top) In an early experiment, researchers used a 10-micrometer-diameter x-ray beam to etch the initials LCLS, about 1.5 millimeters wide, into a piece of boron carbide. (bottom) The team then used an interferometer to assess the depth of the x-ray-induced craters. (Courtesy of SLAC National Accelerator Laboratory.)

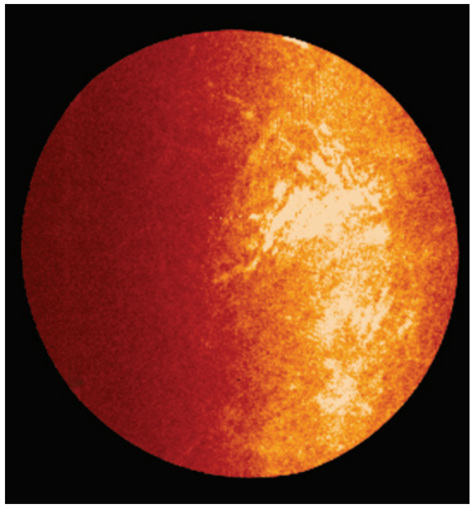
The Real Thing

Following the beam qualification experiments, Hau-Riege led a series of experiments aimed at using LCLS to study equilibrium processes in solid-density plasmas, examine the equation of state of high-energy-density matter, and observe at near atomic scale ultrafast reactions that occur when solids are excited by x rays. The researchers imaged the microstructural lattice of graphite atoms and obtained information about ultrafast order–disorder transformations. "We saw the scattering of the x rays and measured the temperature, density, and distortion before the sample was destroyed," says Hau-Riege.

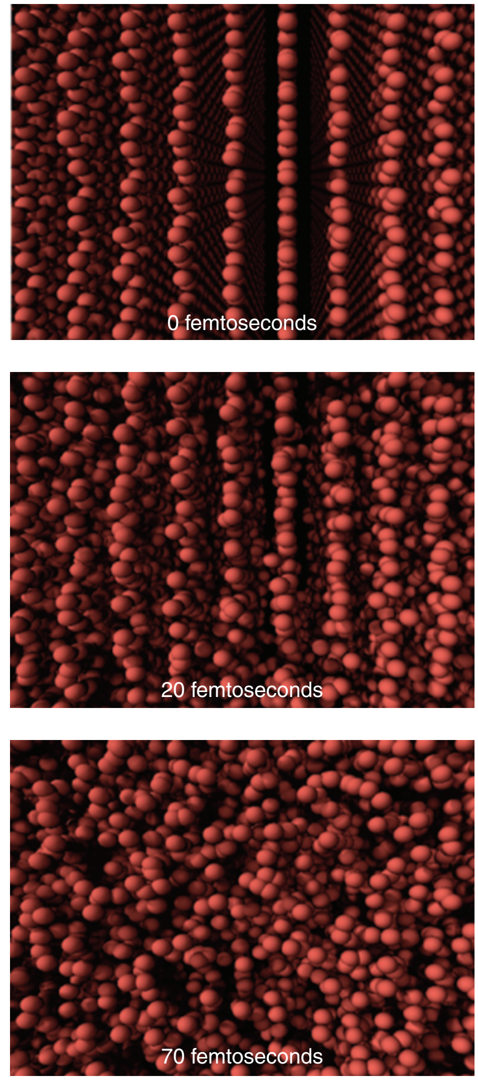
Hau-Riege explains that DOE programs in stockpile stewardship and inertial confinement fusion require high-quality data describing the properties of high-energy-density matter. In particular, data from LCLS experiments will complement those generated by the National Ignition Facility (NIF), the most energetic laser in the world, which is located at Lawrence Livermore. "NIF can create much higher pressure–density regimes than LCLS," he says. NIF, however, operates in ultraviolet wavelengths, and the "very pure" hard x rays from LCLS promise to reveal important details about excited materials to complement data from NIF experiments.

LCLS experiments to date have validated simulations Hau-Riege and other physicists have conducted using Livermore supercomputer codes. For example, LCLS results are compared with Livermore's molecular-dynamics simulation code ddcMD, which is used to model the evolution of hot, dense, radiative burning plasmas. (See the right figure on p. 9.) The experimental results demonstrate the importance of including quantum mechanical processes in these models.





LCLS experiments imaged the diffraction patterns of (left) single-crystal graphite and (right) nanocrystalline graphite. The single crystal measures about 1 centimeter square. The nanocrystalline graphite, of approximately the same size, is composed of many nanocrystals, each measuring about 30 nanometers in size and reconstituted from powder.



Supercomputer simulations guide Livermore experiments on LCLS. In this example, a simulated graphite lattice is shown 20 and 70 femtoseconds after exposure to the laser beam. Experiments on LCLS are largely validating the simulations.

Using One Laser to Create a Second

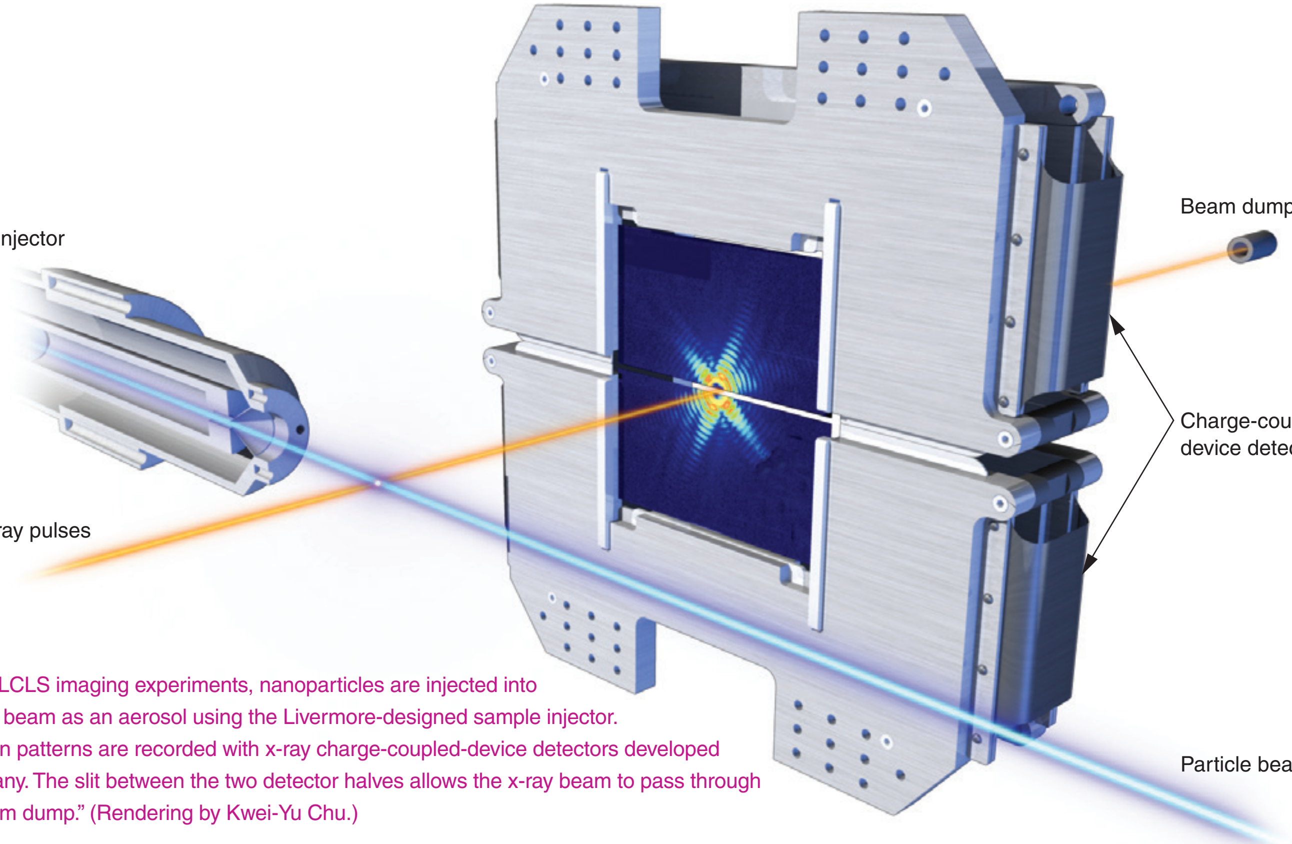
LCLS produces x rays through a process called self-amplified spontaneous emission, which means the x-ray beam is not temporally coherent within each extremely short pulse. Each pulse comprises 50 to 200 temporal spikes of random intensities and phases. Livermore physicist Nina Rohringer and her team have been conducting experiments to create a more temporally coherent atomic x-ray laser that is "pumped" by the LCLS x-ray pulse.

The goal is to use the LCLS beam to eject electrons from an atom's inner shell—only x-ray photons can knock out inner-shell electrons. The "holes" in the inner shell are almost instantaneously replaced by electrons from the atom's outer shell, in the process generating a pulse of hard x rays only a few femtoseconds long. In addition to producing shorter pulses, the secondary x-ray pulse is also considerably smoother than the LCLS x-ray beam. In September 2010, proof-of-principle experiments were conducted with neon gas. "With LCLS acting as a pump, we can create very intense, ultrashort pulses," says Rohringer. The experiments were conducted in collaboration with Livermore's Hau-Riege, Jim Dunn, Richard London, Felicie Albert, Alex Graf, and Randy Hill; Colorado State University's Jorge Rocca, Duncan Ryan, and Mike Purvis; SLAC's John Bozek and Christoph Bostedt; and an LCLS support team.

This type of experiment was first conceived in the 1960s, but x-ray pumping sources were far too weak. In 1984, Livermore physicists developed the first atomic x-ray laser, which was based on powerful optical lasers producing collisions of electrons in hot plasmas. Rohringer says that several scientific communities might benefit from shorter x-ray pulses and improved temporal coherence. For example, shorter pulses could enable studies of chemical reactions or phase transitions in solids, while the longer coherence time would make possible, for the first time, the direct study of nonlinear quantum optics. Broadly applied nonlinear spectroscopic techniques, such as Raman spectroscopy, could be transferred from the optical to the x-ray regime and could result in new, powerful analytical tools to study electronic excitations in solids and molecules in a time-resolved manner.

Imaging Biomolecules

One of the most promising avenues of LCLS research is imaging biomolecules,



In some LCLS imaging experiments, nanoparticles are injected into the x-ray beam as an aerosol using the Livermore-designed sample injector. Diffraction patterns are recorded with x-ray charge-coupled-device detectors developed in Germany. The slit between the two detector halves allows the x-ray beam to pass through to a “beam dump.” (Rendering by Kwei-Yu Chu.)

including proteins, DNA, RNA, and viruses. Much of what scientists know about the detailed structure of biomolecules has come from x-ray diffraction studies of crystalline forms. Researchers traditionally have generated three-dimensional images of large biomolecules with x-ray crystallography, using x rays much weaker than those generated by LCLS. For example, x-ray crystallography was used to elucidate the double-helix structure of DNA. However, at this time, some biomolecules, such as most membrane proteins, cannot be crystallized. Studying the dynamics of noncrystalline structures requires a different x-ray diffraction technique that uses brighter x rays of shorter duration and wavelengths than have been available to date at synchrotron x-ray sources. (See *S&TR,* January/February 2009, pp. 16–18.)

Scientists have long theorized that an ultrashort and extremely bright x-ray pulse could create a single diffraction pattern from a large biomolecule before the x rays destroy the sample. If so, scientists could better understand the structure of proteins without having to crystallize them first. Key challenges have included recording ultrafast, single-shot, coherent diffraction patterns of injected biomolecules with low signal-to-noise ratio and developing robust algorithms to construct images from the diffraction patterns.

Since 2005, Livermore physicist Matthias Frank has been working on x-ray laser experiments as part of a multiyear project funded by Livermore’s Laboratory Directed Research and Development Program. This effort, formerly led by physicist Henry Chapman (now at DESY and the University of Hamburg), aims to validate the idea of using short and intense x-ray pulses to capture images of biomolecules.

In 2006, scientists made history using the FLASH soft x-ray free-electron laser at DESY. A Livermore team, including Frank, Hau-Riege, and Chapman, was part of an international collaboration with colleagues from SLAC, UC Davis, and European institutes that demonstrated how XFELs can image the ultrafast dynamics of nanoscale materials and biological structures. A Livermore-developed computer algorithm re-created an image of the object based on the recorded diffraction pattern. The Livermore team conducted additional experiments at FLASH over the next three years, gaining confidence that LCLS, when it began operation, could successfully capture images of biological materials and eventually reveal protein structure.

More recently, working with researchers from DESY, Max Planck Institute, and Arizona State University, Frank and other Livermore scientists participated in experiments in which LCLS x-ray pulses, operating at 2 kiloelectronvolts and a 6-nanometer wavelength, were used to image crystalline biological materials measuring a few nanometers in diameter. Because the AMO end-station is not designed for imaging biomolecules, the German researchers brought their own experimental chamber equipped with x-ray cameras developed at the Max Planck Institute. The chamber was bolted to the back of the end-station.

According to Frank, the biological imaging technique is revealing the structure of proteins and determining how they interact with other biomolecules. (See *S&TR*, May 2007, pp. 21–23.) Proteins are complex macromolecules that range from 400 to 27,000 amino acids in length, and their structures are a tangle of folds and twists. These structures may shift several times during their normal biological functions. Determining a protein's three-dimensional structure provides important clues about its behavior and function and guides the development of new drugs. While x-ray crystallography has revealed many secrets of protein structure, data from LCLS experiments with single molecules promise to reveal many more. UC is currently funding Frank and collaborators from UC Davis to apply x-ray imaging at LCLS to several biological molecules of interest.

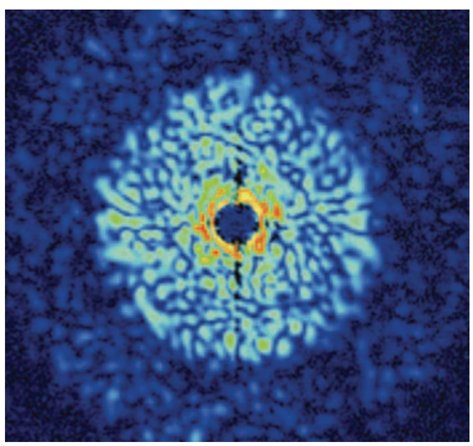
Frank notes that experimentalists at LCLS will soon have the option of triggering an optical laser to fire at a sample shortly before an x-ray pulse with an adjustable time delay. Such a pump-probe technique could prove valuable as a way to determine if a protein changes shape when exposed to light.

SLAC funded Frank to help develop a particle injector for the coherent x-ray imaging instrument. The instrument, which was commissioned in November 2010, is designed to image single nanoparticles, such as biological macromolecules, that are not in crystalline form. "We need to deliver nanoparticles or macromolecules from a sample into the LCLS vacuum chamber at a high rate and into exactly the right place," he says. Frank and coworkers developed an injector based on a design previously used at Livermore for single-particle aerosol mass spectrometry, which sucks ambient particles such as bacteria and viruses into a mass spectrometer to identify single particles for biodefense and environmental monitoring.

The new sample injector produces a tightly focused stream of nanoparticles aimed into the path of the incoming x-ray pulses, which hit particles on the fly. X rays scattering off atoms in the sample particle produce a diffraction pattern revealing the particle's structure. Because the incoming x-ray pulse is so short, this diffraction pattern is produced just before the molecule explodes from the energy absorbed. The procedure is repeated many times a minute. Diffraction patterns from several individual particles can be measured each second, and thousands to hundreds of thousands of patterns are recorded in a single experiment. Even with the same type of molecule, the diffraction patterns differ because atoms and molecules are in constant motion and face the beam in different orientations. A single three-dimensional image of a representative molecule is constructed from terabytes of data consisting of many thousands of two-dimensional diffraction patterns.

At LCLS, two experimental halls will eventually house six chambers for research in atomic–molecular physics, pump-probe dynamics of materials and chemical processes, x-ray imaging of clusters and complex molecules, and plasma physics. Hau-Riege says the light source is working with little downtime compared to other facilities during their startup phase. "It is extremely stable, and the beam is easy to align." He notes that it has become highly competitive to obtain experimental time on the machine as word spreads among the scientific community of LCLS's extraordinary x-ray beam qualities.

—*Arnie Heller*



An experiment at the FLASH soft x-ray free-electron laser at Deutsches Elektronen-Synchrotron in Hamburg, Germany, generated an x-ray diffraction pattern from a single 1-micrometer soot particle. Similar experiments are being performed on LCLS.

Key Words: FLASH laser, Linac Coherent Light Source (LCLS), nanoparticles, proteins, self-amplified spontaneous emission, single-particle aerosol mass spectrometry, SLAC National Accelerator Laboratory, x-ray free-electron laser (XFEL).

For further information contact Stefan Hau-Riege (925) 422-5892 (hauriege1@llnl.gov).

From Data to Discovery

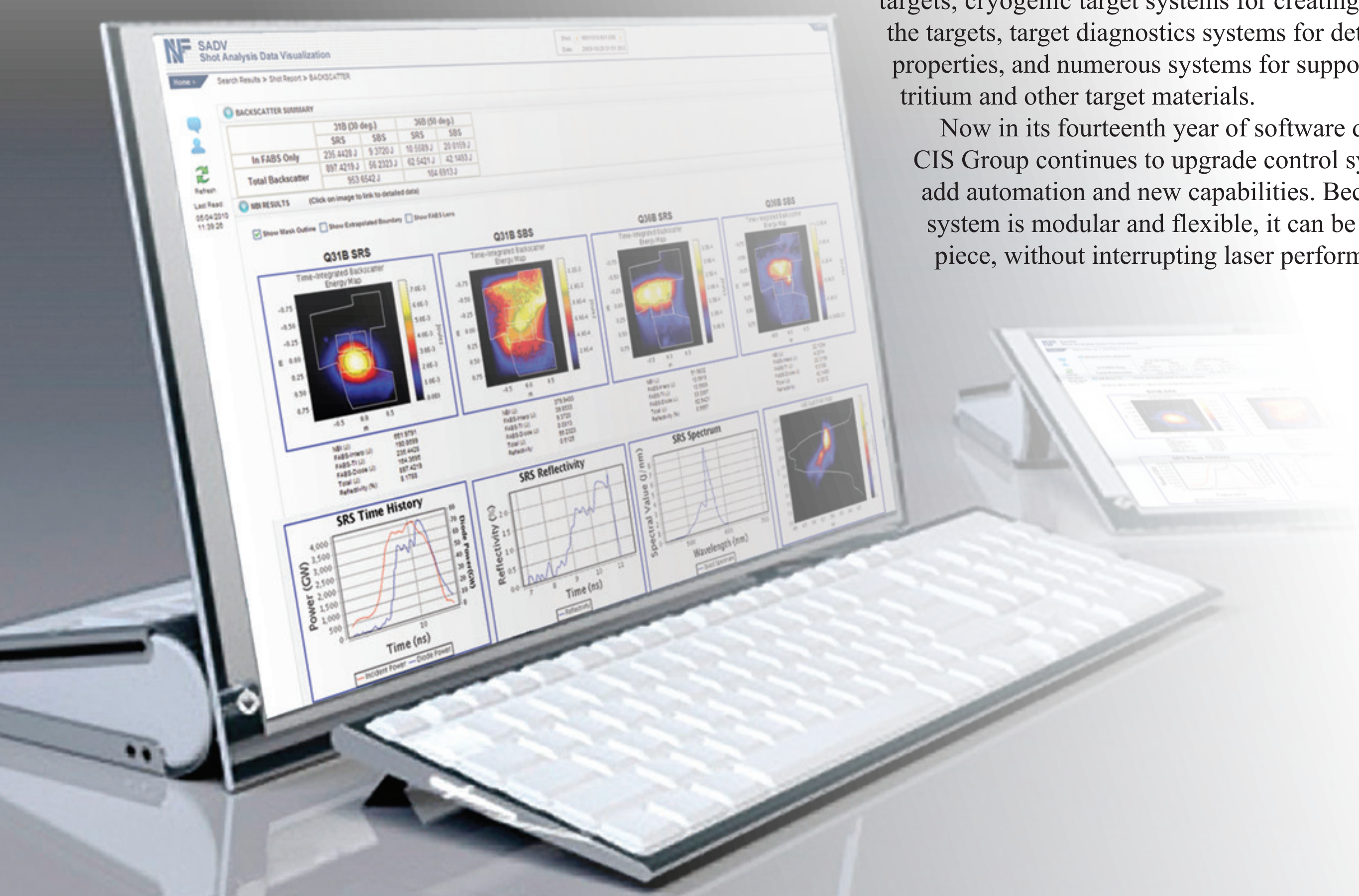
HOW do you design a computer system that will be relevant and useful for decades? For computer architects developing the control system for Lawrence Livermore's National Ignition Facility (NIF), the central nervous system of the world's largest and most energetic laser, the solution centered on designing flexibility into the system from the beginning. The size of three football fields and 60 times more powerful than any other laser, NIF was declared fully operational in March 2009. It is run by the most complex, real-time control system ever designed for scientific research, a system that is intimately involved in all aspects of NIF's performance and maintenance.

The behind-the-scenes workhorse, the integrated computer control system (ICCS), was designed and developed by NIF's Controls and Information Systems (CIS) Group. Paul Van Arsdall and Larry Lagin lead the team of about 200 developers, engineers, technicians, information technology specialists, and quality control experts. According to Lagin, a 30-year fusion technology veteran, the key attribute of the control system is its dynamic, flexible design. Both the design of ICCS and the goals of the CIS Group have had to be flexible to meet the facility's evolving needs and to support its users. The original focus of control system software and hardware development was building functionality to enable NIF to successfully meet its milestones throughout the construction project.

Aiming for Automation and Flexibility

The controls effort has shifted over the last several years to developing software for automating experiments. That software, originally deployed to automate shots to commission the laser, has been expanded to control the full range of experiments planned for the National Ignition Campaign. Capabilities added to the control system over the past year include positioner control for aligning targets, cryogenic target systems for creating ice layers inside the targets, target diagnostics systems for determining reaction properties, and numerous systems for supporting the use of tritium and other target materials.

Now in its fourteenth year of software deployment, the CIS Group continues to upgrade control system software and add automation and new capabilities. Because the control system is modular and flexible, it can be upgraded piece by piece, without interrupting laser performance. Early on,



In the NIF Control Room, which is modeled after the National Aeronautics and Space Administration's mission control room, operations staff members interact with the "supervisory" portion of the control system. The sophisticated system is designed to use manual control and automation as applicable.

the CIS Group chose CORBA middleware as the architecture that communicates among various hardware and software platforms across the control system. According to Lagin, CORBA has proved to be flexible. "We can now upgrade languages and our computers because we chose CORBA," he says. Ada, the primary software language within the processors that interface with motors and other laser and target equipment, is no longer a common language choice. This change has prompted CIS engineers to gradually migrate to Java, a current industry-standard language that offers excellent diagnostic and development tools and can run on many types of operating systems. Because CORBA allows disparate languages to talk to one another, having some components in Ada and others in Java during the gradual migration is easily accommodated. The software language migration is just one aspect of the ongoing control system software and hardware maintenance effort that happens behind the scenes.

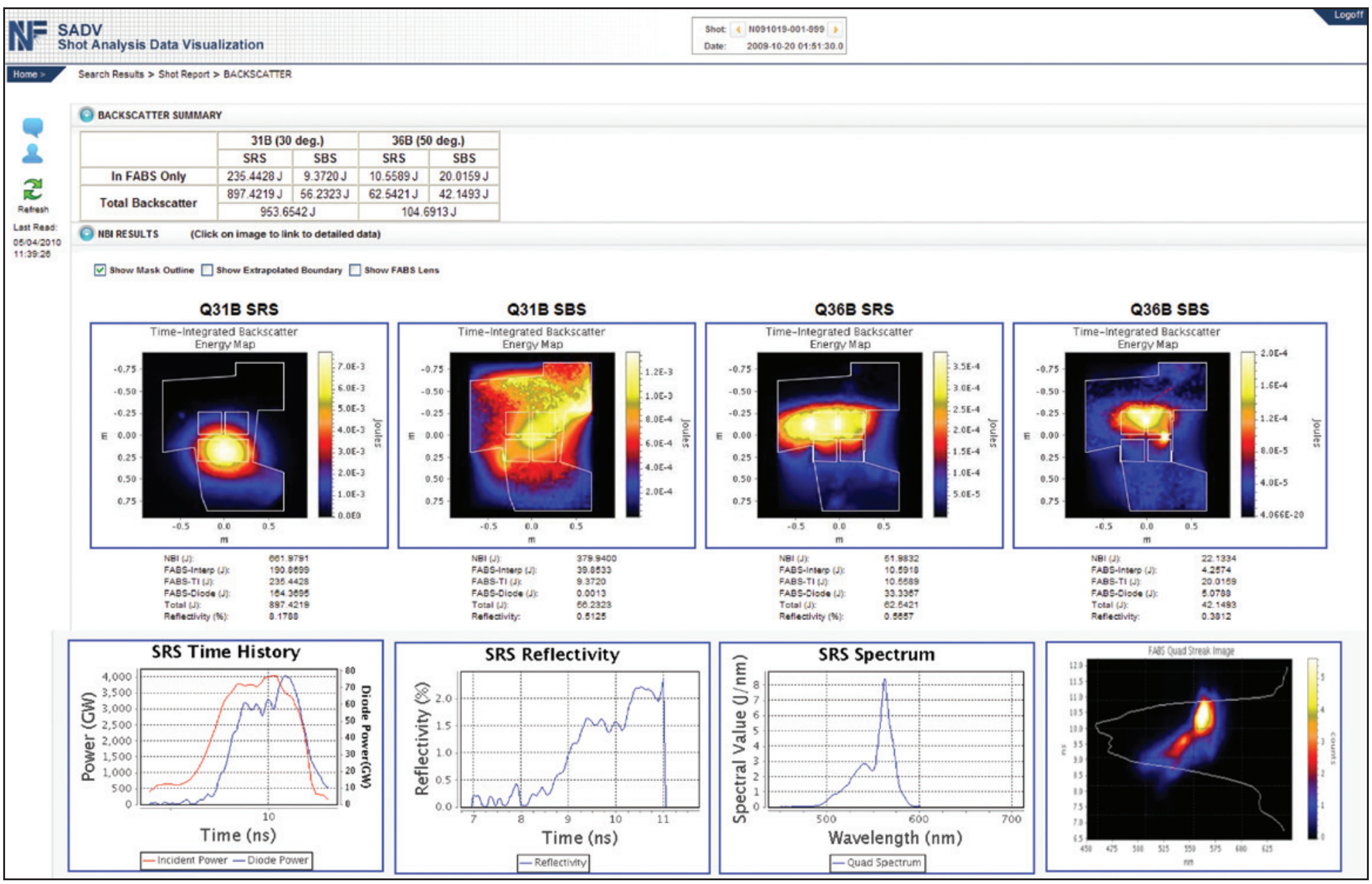
As NIF moves toward full operation as a scientific user facility with an anticipated 30-year lifespan, the CIS Group also is endeavoring to increase the number of tools that will support science experiments and meet the needs of current and future NIF users. Ric Beeler leads a team that has been expanding and improving these tools. Scientists performing an experiment at NIF first interact with campaign management tools, a suite of software applications designed to translate experimental plans and specifications into actions for the control system. After a shot, scientists use the shot analysis, visualization, and infrastructure (SAVI) tools to archive, analyze, and view the experimental results. While a version of the campaign management tools has existed since early experiments were performed in 2003 with just four of NIF's 192 beams, the system is much more sophisticated now. "The management tools have grown up with the control system," says Beeler. Several tools have recently been added to the suite to help scientists more effectively set up their desired shots.

Mining Experimental Data for Gems

The speed and power of NIF's 192 laser beams converging on and bombarding a tiny target with massive energy may inspire wonder, but what happens after a NIF experiment is no less crucial to advancing science and energy research. Managing, organizing, and storing the flow of data from these experiments is no small task. Ten terabytes of experimental data, in multiple formats and from various sources, are generated each month, an amount equivalent to the entire printed collection of the U.S. Library of Congress. Data generation actually begins before a laser shot. Information is captured about the initial condition of each experiment, including the precise shape of the target capsule and the thickness of ice layers within a cryogenic target. (See *S&TR*, June 2010, pp. 17–19.) Immediately after a laser shot, SAVI automatically records, processes, and refines much of the raw data produced by the dozens of x-ray, nuclear, and optical diagnostics that measure aspects of the experiment. (See *S&TR*, December 2010, pp. 12–18.)

The SAVI tools were developed in close collaboration with scientists who perform target experiments to determine how the software tools could best support NIF users. SAVI archives all of the target diagnostic data that are captured electronically by ICCS. A portion of the archived data is processed through the SAVI analysis pipeline, while the remaining data are made available to scientists for use in their analysis applications. The SAVI analysis engine processes information at three hierarchical levels representing the steps in the analysis flow: instrument, diagnostic, and campaign. For example, at the instrument level, SAVI will provide results from an individual hardware device, such as a camera, adjusting for instrument performance factors such as nonlinear gains. At the campaign level, it will refine and combine data from several diagnostics to determine overall characteristics of the experiment such as radiation temperature.

SAVI data visualization tools help scientists view and understand the experimental results. Within these Web applications, scientists can choose to view the raw data or any level of the analysis. Researchers want to access experimental data soon after a laser shot, with the minimum likelihood of error. They use some of these data to determine parameters for the next shot in a series, which might occur just a few hours later. SAVI tools provide experimental results within 30 minutes of a shot through a Web interface, with error bounds and quality metrics. Scientists can review the data remotely or locally, download results, and perform and upload their own analysis.



The shot analysis, visualization, and infrastructure tools help scientists quickly view and interpret data from a just-completed NIF experiment.

Tim Frazier inspects control system servers that run applications for recording and processing shot data. Frazier led the development of the NIF experimental data repository, which captures and stores the data produced by each laser shot.

Safeguarding Results for Years to Come

Experimental data, plus data on the postshot state of the facility, are housed in and retrieved from the NIF data repository. This archive, designed over the past few years, stores all the relevant experiment information—including target images, diagnostic data, and facility equipment inspections—for 30 years using a combination of high-performance databases and archival tapes. Although most scientists analyze data and publish results shortly after an experiment, retaining the data will allow researchers to retroactively analyze and interpret results as scientific fields advance and theories change, or perhaps to build on experimental data originally produced by other scientists.

The intention is to eventually make much of the unclassified data available to the scientific community at large. Beeler notes that this wealth of stored experimental data will make the archive "a real treasure." The staff maintaining the archive faces the ongoing challenge of keeping the archive's hardware and software modern, functional, and relevant. "It's a constant race to keep up to date but still maintain a stable system," says Tim Frazier, head of NIF Information Technology and the data architect who led the development of NIF data storage capabilities.

A crucial design feature of the database, from a scientist's point of view, is preserving the pedigree of the data. Frazier likens the data pedigree to a family tree that traces members and relationships through time. With science data, the "family members" are all the linked pieces of information from a particular experiment such as algorithms, equipment calibrations, configurations, images, and raw and processed data. If it were discovered months after an experiment that a camera was miscalibrated, for example, the correction could be entered into the data set, and all of the family members, or linked pieces of data that feed from or rely on that calculation, would be overlain by new, corrected versions. Having a long-term record of this linked, versioned data is invaluable to scientists as proof of the validity of their results.

The database relies on both commercial Oracle software and open-source technology. What sets it apart from other large scientific data archives, such as that of CERN (the European Organization for Nuclear Research), is that both structured and unstructured data reside inside the database. By bringing images and other raw, unstructured content into the database, CIS staff can use one tool set and one skilled team to back up and manage the data. According to Frazier, being able to handle these "blobs" of data is a fortunate matter of timing; the database was designed and built at a point where computer technology was fast and powerful enough to handle both raw and processed data files within one archive.

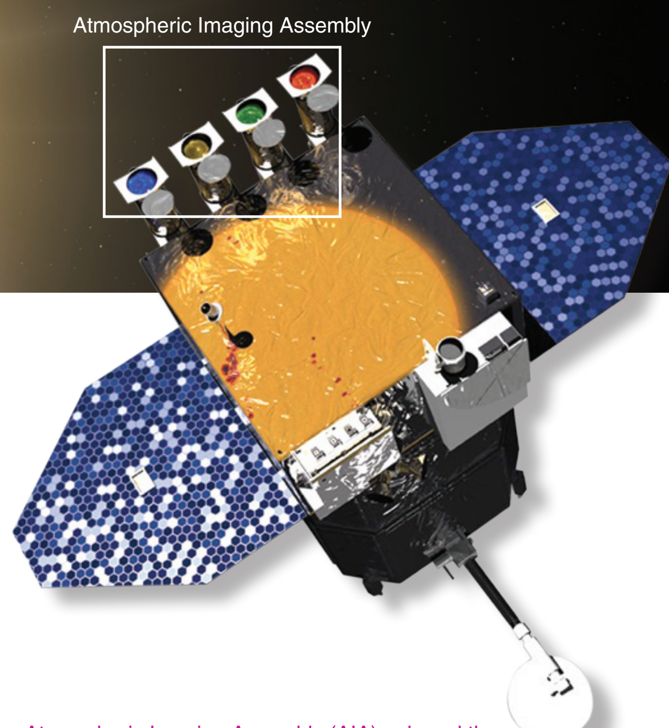
The control and information systems consist of more than 2,000 computers, terabytes of data, and plentiful software tools, all working together to produce, record, and process experimental information. As Frazier emphasizes, NIF is a marvel, but its purpose is simple. "NIF is an incredible data-generating machine," he says. "What really matters are the data and the scientific understanding that evolves from this information." Handling, processing, and storing experimental data for scientists to use and mine for new discoveries is a crucial charge for CIS staff, one that enables and supports the work of experimentalists. From these vast records made up of ones and zeroes will likely come groundbreaking discoveries and evidence to advance fusion research and many other areas of science.

—*Rose Hansen*

Key Words: campaign management tools; CORBA; computer automation; data archive; integrated computer control system (ICCS); National Ignition Facility (NIF); shot analysis, visualization, and infrastructure (SAVI).

For further information contact Trish Damkroger (925) 422-5816 (damkroger1@llnl.gov).

The Sun in All Its Splendor



The Atmospheric Imaging Assembly (AIA) onboard the Solar Dynamics Observatory (SDO) is a suite of four telescopes that image seven wavelengths of extreme ultraviolet light emitted from the Sun. (Courtesy of the National Aeronautics and Space Administration [NASA].)

THE Sun is the lifeblood of our planet. It provides the light, heat, and energy to Earth that is essential for perpetuating the existence of all living things. But as important as this star is, relatively little is known about its physical processes and often-volatile behavior. On February 11, 2010, the National Aeronautics and Space Administration sent the Solar Dynamics Observatory (SDO) into orbit to capture the highest temporal and spatial resolution, full-disk images of the Sun ever acquired. By studying the solar corona in more detail, researchers expect to learn more about the Sun's magnetic field, enabling them to better understand solar events that can adversely affect satellite communications, power grids, and many other aspects of life on Earth.

Onboard SDO is the Atmospheric Imaging Assembly (AIA), a suite of four telescopes that contain highly reflective multilayer mirrors codeveloped at Livermore. These sophisticated optics consist of two materials layered in a repeating sequence on top of a mirror substrate and allow AIA to image the Sun at seven wavelengths of extreme ultraviolet (EUV) light. Each EUV wavelength corresponds to an emission line of ionized solar materials (iron or helium) at different temperatures. AIA images all seven EUV wavelengths (and three additional ultraviolet and visible wavelengths) every 10 seconds to create "snapshots" of distinct features within the Sun's atmosphere at a resolution 10 times greater than that produced on a high-definition television. The AIA project at Livermore was funded by the Smithsonian Astrophysical Observatory, and the AIA principal investigating institution is Lockheed Martin Solar and Astrophysics Laboratory in Palo Alto, California.

Deposition of multilayer thin films was first attempted in the 1940s, but the technology of the time and the choice of materials were inadequate to create layers that would maintain stable interfaces when stacked one on top of the other. Three decades later, the first viable multilayer coatings were developed. Soon after, Livermore researchers became leaders in advancing multilayer thin-film coatings for a variety of physics applications and for EUV lithography, a technology that uses reflective multilayer mirrors for manufacturing improved computer chips. (See *S&TR*, October 2003, pp. 8–9.) Says Livermore physicist Regina Soufli, who led the Laboratory's SDO optic development team, "The improved multilayer mirror technologies created during our pursuit of EUV lithography made the SDO optics possible."

A Material Worth "Bragging" About

EUV wavelengths range between 50 and 5 nanometers, which coincide with the characteristic absorption wavelengths of inner-shell electrons in the atoms that compose matter. As a result, EUV light directed onto a standard mirror or lens at normal incidence is absorbed rather than reflected, making it undetectable. For this reason, EUV light is also absorbed by Earth's atmosphere, which is why telescopes must travel to space to study the light emitted from the Sun.

Multilayer mirrors achieve high reflective performance by acting as synthetic Bragg crystals. This effect is created by layers of materials deposited in a periodic stack. Through constructive interference of the reflected electric fields across the layers, these structures can efficiently reflect radiation at specific wavelengths according to Bragg's law, a formula that relates the reflected wavelength to the angle of the incident light and the periodic thickness of the individual layers. "For example," says Soufli, "we used a structure made from 50 molybdenum–silicon bilayers, each a few nanometers thick, to achieve optimum optical contrast and thus the highest reflectivity for EUV light at normal incidence."

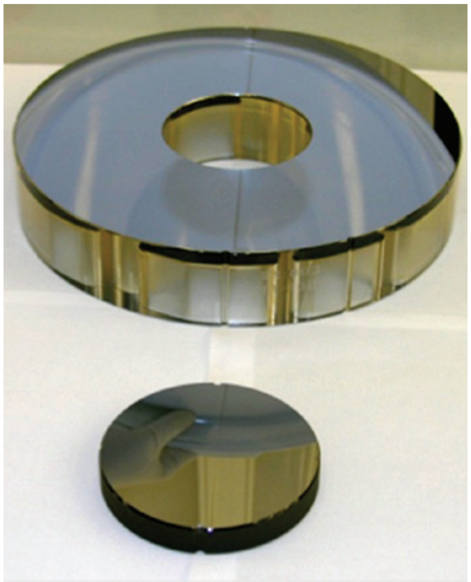
Silicon and molybdenum are one of the few material combinations that can produce the right contrast for the solar wavelengths of interest on SDO. This material pair also has a history of stability, durability, and reliability in EUV-related applications, which made it an obvious choice for four of the SDO EUV wavelengths. Collaborators from Reflective X-Ray Optics, LLC, in New York City, used other material combinations as well, such as molybdenum–yttrium and silicon carbide–silicon to create multilayer coatings for the other three SDO EUV wavelengths.

The Laboratory team, which includes Soufli, Eberhard Spiller, Jeff Robinson, Sherry Baker, and Jay Ayers, used a magnetron sputtering deposition system combined with a velocity modulation technique to achieve the precision SDO multilayer coatings. (See *S&TR*, October 2002, pp. 10–11.) By adjusting the bilayer thickness in the multilayer coating, researchers can "tune" each mirror to selectively reflect a specific EUV wavelength of solar radiation.

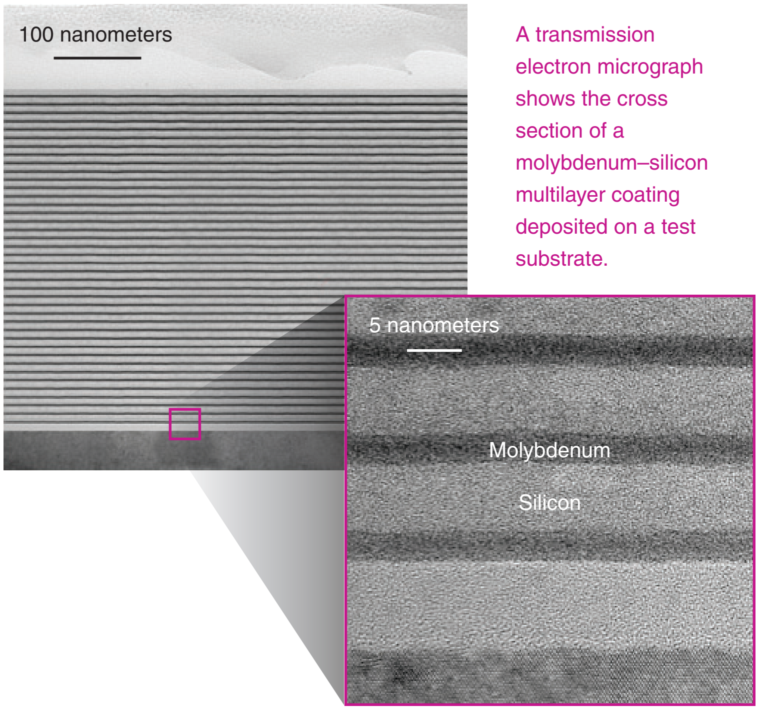
Overcoming Obstacles

Each of the four AIA telescopes contains a primary and secondary curved mirror designed to reflect light at two wavelengths. Two different reflective multilayer coatings must be deposited on each D-shaped "half" of the circular mirror substrate's front surface to achieve this result. Each coating acts as a reflective filter that separates the desired EUV wavelength from other visible, ultraviolet, and EUV light emitted from the Sun. Light entering the telescope reflects off the larger, concave primary optic (200 millimeters in diameter) onto the convex secondary optic (80 millimeters in diameter), which then reflects the light back through a small hole in the center of the primary optic. A detector behind this mirror measures and records the light for imaging.

The Livermore team had to overcome several challenges to create the multilayer optics with the precision and quality needed for SDO. A major task was trying to create a uniform layer of material across the curved surface of the optic. "Each multilayer coating must reflect at the same wavelength (to within a couple percent) across the entire curved mirror segment," says Soufli. "The challenge was to control the deposition process in a way that achieves a layer of constant thickness across the concave or



The four AIA telescopes each contain a large primary concave mirror (200 millimeters in diameter) and a smaller, secondary convex mirror (80 millimeters in diameter). Each mirror assembly can reflect light at two wavelengths.



A transmission electron micrograph shows the cross section of a molybdenum–silicon multilayer coating deposited on a test substrate.

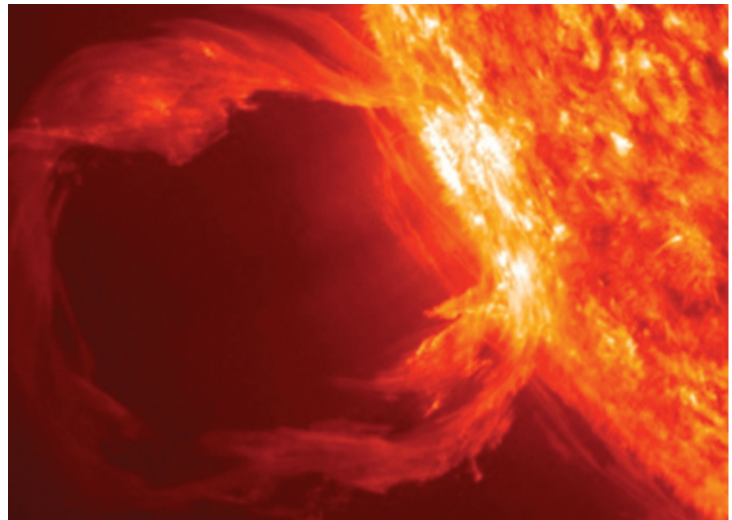
convex mirror surface. If the layer thickness differed from the desired specification by more than one-tenth of a nanometer, the SDO images would be degraded." During deposition, the velocity modulation technique allows for precise control of the multilayer thickness to compensate for the curvature of the optic. Using a custom-developed algorithm, researchers can adjust the speed of the deposition platter that holds the optic as it passes under the sputtering materials to achieve the desired thickness.

Additionally, because the multilayer coating could be deposited only over one-half of the optic at a time, the team needed a way to prevent material from being deposited on the other half of the optic and to minimize the area across the middle where the two coatings overlap. The solution was an optimized hardware mask that covers half of the circular optic as the other side is being coated. "We had to get the mask as close to the mirror surface as possible without actually touching it," says Soufli.

During deposition, particles from the sputtered material can bounce off the edge of the mask and land near and under it, an effect that is referred to as "shadowing." The area on the optic affected by shadowing, which includes the region where the two coatings overlap, does not reflect EUV light efficiently. "Think of the mask as an awning attached to a house during a rain storm," says Soufli. In this situation, most of the area underneath the awning will remain protected, but a few drops will land under the covering. "We engineered the mask to minimize detrimental shadowing effects on the area being coated, thus greatly improving the performance of the SDO multilayer optics."

The substrates onboard SDO were fabricated of ZERODUR® glass material and polished by commercial vendors. Each flight substrate, prior to multilayer deposition, was inspected by the Livermore researchers using atomic force microscopy. This technique enabled them to determine the substrate's surface roughness and other possible defects that could diminish reflective performance.

Before the finished optics were installed, the reflective performance was measured using the reflectometer facility on Beamline 6.3.2 at the Advanced Light Source, which is operated by the Center for X-Ray Optics at Lawrence Berkeley National Laboratory. "The peak EUV wavelength and reflectivity were measured at several locations across the surface of each mirror, thus creating 'maps' of the mirrors' experimental performance as they would operate onboard SDO," says Soufli. These calibration tests provided essential data that make it possible to accurately interpret the data transmitted by the AIA instrument.



SDO is enabling scientists to capture impressively high-resolution images of the Sun's physical processes. For example, this image shows a prominence eruption, which corresponds to an extreme ultraviolet emission line of ionized helium. (Courtesy of NASA.)

A Hot Topic

Over the course of SDO's five-year mission, scientists will use the collected images of the Sun to better understand space weather, for example, how the Sun's magnetic field contributes to activity such as solar flares and coronal mass ejections. By studying the Sun's physical processes in greater detail, scientists can improve predictions of solar activity, which can aid in protecting spacecraft crews as well as Earth's electrical and communications infrastructure. Equipped with Livermore's precision multilayer mirror technology, SDO is illuminating the Sun's inner workings and outward manifestations of those processes to provide essential data about Earth's most important star.

—Caryn Meissner

Key Words: Advanced Light Source, Atmospheric Imaging Assembly (AIA), extreme ultraviolet (EUV) light, magnetic field, magnetron sputtering deposition, multilayer mirror, solar corona, Solar Dynamics Observatory (SDO), solar physics, Sun.

For further information contact Regina Soufli (925) 422-6013 (soufli1@llnl.gov).

Drilling Deep into Plant Veins

WHAT cows do quite naturally does not come so easily for humans. Termites and ruminants such as cows digest cellulose—the main component of woody material in plants—with the aid of gut microorganisms, but scientists struggle to efficiently perform the same task for biofuel production. Researchers want to exploit cellulose, the most abundant organic material on Earth, from wood, grasses, or plant waste materials to create fuels to power our cars and cities. The crucial step in the biofuel production process is efficiently breaking down the long chains of sugars that comprise cellulose into simple sugars. This process has proved both challenging and expensive because of the complex structure of cellulose-yielding plants. *Zinnia elegans* is an annual plant with exuberant flowers and lacy leaves—not anyone's idea of a green waste material. But the garden-variety zinnia's lacy leaves have been put under the microscope in an effort to visualize plant cell structure and eventually develop more efficient ways to extract the raw ingredients for biofuels.

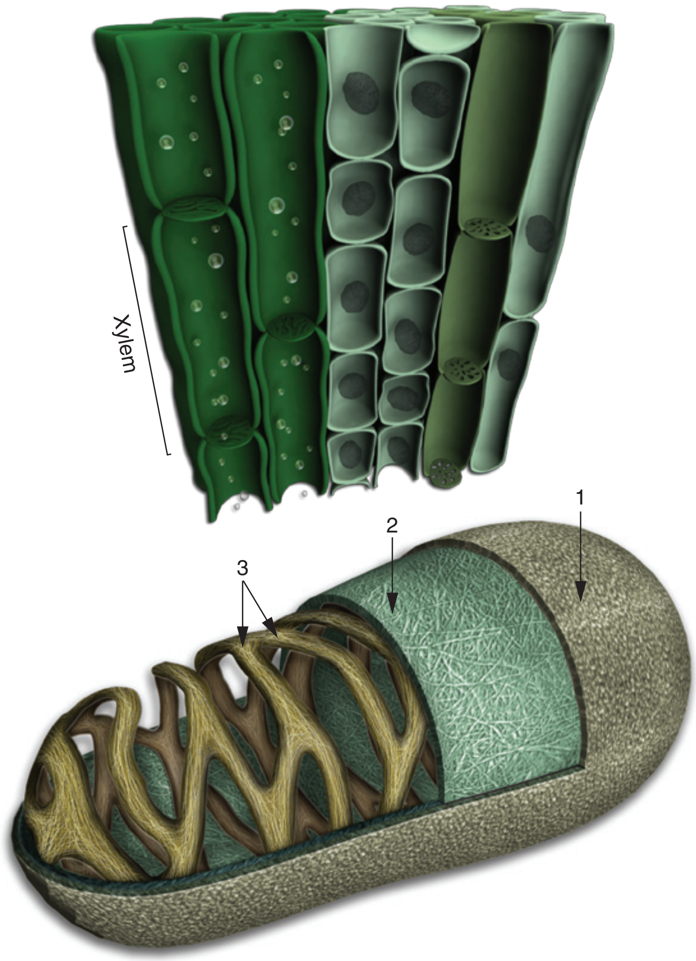
A team led by Livermore scientist Michael Thelen, in collaboration with scientists at Lawrence Berkeley National Laboratory and the National Renewable Energy Laboratory (NREL), uses a novel combination of imaging techniques to view the supportive structure of zinnia leaf cells at several length scales and to observe changes during the deconstruction of cellulose-yielding cells. The structure of supportive cellular elements in plants is rather poorly known, so this work has applications both to basic plant science and to biofuel production. According to Thelen, "We look at the heart of what makes up the woody materials in plants for use in biofuels." While other research groups also study how to break down cellulose in plant tissues, this work differs because it uses single plant cells to fundamentally understand the initial stages of deconstruction.

Targeting Transformed Cells

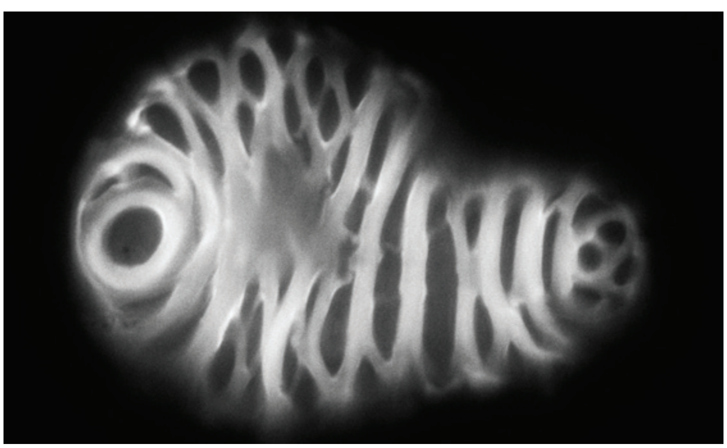
Plant scientists noted several decades ago that mesophyll cells (the primary site for photosynthesis) harvested from the leaves of zinnia seedlings will transform into xylem cells (the principal water-conducting tissue of vascular plants) when cultured in liquid for several days and exposed to plant hormones. Says Thelen, "Scientists previously have found that leaf cells in culture can be induced to give rise to structures and processes that normally happen in nearby, but different, cells."

Mesophyll cells that transdifferentiate into xylem, or woody, cells have created a highly supportive secondary cell wall consisting mostly of cellulose, in organized patterns of hoops, spirals, or reticulated networks. Near the end of this process, lignin deposits form, and then the cells undergo a programmed death, leaving behind only their shells. In plants, these "functional corpses," as they are sometimes known, are linked end to end to form the sturdy, water-transporting veins that link the roots to the leaves of plants. "Those hollow shells made of cellulose and the lignin that sheaths it are the crucial part of the plant we are studying," says Thelen. "They contain 70 percent of the lignocellulose in plants potentially available for biofuels processing."

After isolating leaf cells and inducing secondary cell-wall formation, Thelen's team applied a combination of imaging techniques to both primary and secondary cell walls to characterize their structure and their chemical composition. The structure



Researchers studied a zinnia xylem cell using a combination of imaging techniques. (top) Xylem cells link end to end in a plant to transport water. (bottom) The team observed three main layers in the xylem cell wall: (1) the outer granular matrix, (2) the primary cell wall, and (3) the secondary cell wall. (Rendering by Sabrina Fletcher.)



With fluorescence microscopy, the team observed that autofluorescent components of the xylem cell's secondary wall make the wall's hoops and swirls readily apparent.

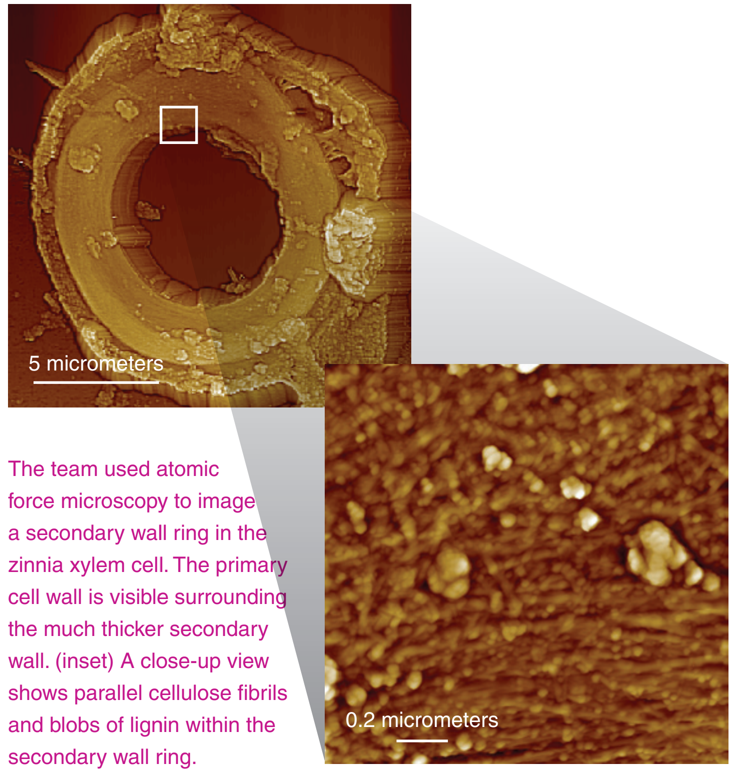
of plant cells varies both by plant and cell type, so the team chose a single type of zinnia cell as a model system. According to Catherine Lacayo, a Livermore postdoctoral researcher who performed much of the hands-on work, this particular zinnia cell is known to perform the synchronized transdifferentiation process in culture. It is also easy to isolate and can produce large amounts of cellulose for its size. Lacayo notes that the team's work can be considered a starting point for industry-oriented biofuels research. "Zinnia is not practical for use beyond a research setting," she says. "The results will be applied to study other plant types—those plants known as feedstocks for biofuels."

A goal of this study was to gain a better understanding of how lignin and cellulose interact chemically and structurally within the secondary cell wall. Both primary and secondary cell walls contain a crystalline mesh of cellulose fibers that strengthen and support the cell and the overall plant. The secondary cell wall contains more cellulose but also lignin, a complex aromatic polymer. Lignin is an obstacle for biofuels scientists because the polymer makes it difficult to access and separate the cellulose targeted for biofuel production. "Lignin is linked to the cellulose fibers through chemical bonding," says Lacayo. Not only are lignin and cellulose chemically bonded, but lignin also is highly hydrophobic and resistant to breakage. Both are essential properties for a substance that lines the water-carrying veins of plants but pose challenges for deconstruction.

Zooming in for a Better Look

Thelen's group used three imaging platforms to study the zinnia cell-wall structures at different scales, which helped to visualize their organization and composition down to the nanometer scale. The structures under study are tiny, although they are about average in the world of plant cells. Generally, each secondary cell wall is 2 micrometers thick, and the xylem cells themselves are just 40 micrometers in length. For all three techniques, cells were divided into two groups. Cells in one group were examined in as close to their natural form as possible. Cells in the other group were chemically treated to strip off lignin and other materials before imaging.

Lacayo used fluorescence microscopy to peer inside the cells at the broadest scale. Ideally, for this imaging technique, the secondary walls in these cells will be highly autofluorescent because of their lignin content, making the hoops and swirls of the secondary cell wall easily discernable. To enhance visibility, Lacayo added to individual cells an NREL-engineered fluorescent protein that binds to cellulose. The cellulose-binding protein worked better when the cells were exposed to hot, acidified chlorite—a chemical treatment used to remove lignin and sugars from the wall. Lacayo explains, "We found that when lignin and some sugars are removed from the cell wall, cellulose becomes more accessible, which was confirmed using atomic force microscopy."



The team used atomic force microscopy to image a secondary wall ring in the zinnia xylem cell. The primary cell wall is visible surrounding the much thicker secondary wall. (inset) A close-up view shows parallel cellulose fibrils and blobs of lignin within the secondary wall ring.

The Livermore team used atomic force microscopy (AFM) to study the cell-wall surface and structures in finer detail. Funding for developing this capability was provided by the Laboratory Directed Research and Development Program. AFM is an imaging and measuring technique, where information is gathered by "feeling" the surface with a mechanical probe. The researchers determined that a granular material with structures a few tens of nanometers thick covers the outer surface of the cells. Drilling down a bit deeper, cells treated with hot, acidified chlorite and imaged with AFM revealed a networked structure of cellulose fibrils comprising the primary cell wall. By breaking the cells apart, they obtained fragments of the secondary cell wall to image as well. These fragments consisted of granular deposits of lignin within cellulose fibrils arranged in parallel. The fibrils were observed to sometimes form thicker groupings up to 100 nanometers wide. These direct observations allowed Thelen's group to develop a model of the zinnia cell-wall architecture. According to Alexander Malkin, a Livermore scientist who lent his AFM expertise to the project, "This is the first time that high-resolution imaging has been done of several structural layers of a cell wall."

Imaging at the most minute scale was performed for the project by Lawrence Berkeley scientist Hoi-Ying Holman. Using synchrotron radiation Fourier-transform infrared (SR-FTIR) spectromicroscopy, Holman looked at the chemical composition of individual cells. Spectromicroscopy identifies and measures substances through the spectrum those substances emit or absorb. Once the cells were treated with chemicals to remove components from the cell walls, SR-FTIR was used to image cell composition. In recorded changes in the relevant absorbance spectra, SR-FTIR imaging showed that the cellulose remaining in each cell was more accessible after lignin was removed with the acidified chlorite treatment.

Platform for Research Growth

The results from this trio of cell imaging techniques are likely to benefit plant biologists and biofuels scientists alike. The Livermore team and collaborators have emerged with a better understanding of the fine structure of the zinnia xylem cell walls, especially the structure of the secondary cell wall with and without lignin. They have developed a chemical and structural model of cell walls and have gained insight into the deconstruction and removal of cell-wall components. By demonstrating a comprehensive and effective combination of imaging techniques on plant cell structures, the researchers have established a new standard in their field.

The Department of Energy (DOE) Genome Science Program and the DOE Joint BioEnergy Institute (a six-institution partnership led by Lawrence Berkeley in which Thelen is also involved) have supported this work as part of a larger research effort to turn biomass into fuels using microbial enzymes. For Thelen's group, research continues. Building on what they have learned, the Livermore scientists are now working on imaging the deconstruction of zinnia cell walls using various enzymes extracted from microbes. "Our goal is to systematically break down the plant cell wall and to monitor that process using high-resolution imaging in real time," Lacayo says. The next step will likely be to select microbes with desirable characteristics, such as adaptability to high temperatures, and study how effectively each particular microbe's enzymes break down cellulose and other sugars.

The successful characterization of the zinnia cell-wall structures has provided a more comprehensive understanding of the supportive structures comprising zinnia leaf veins and how decomposition of complex sugars occurs in these regions. But perhaps most importantly, Thelen's group has discovered a winning combination of techniques to peer deep within a cell, a research platform that will likely prove useful to many other plant scientists. Biofuels scientists, too, may benefit from the brilliantly hued zinnia plant, which is helping to unlock the secrets to plant cell-wall construction and deconstruction.

—Rose Hansen

Key Words: atomic force microscopy (AFM), biofuel, cellulose, fluorescence microscopy, Joint BioEnergy Institute, lignin, lignocellulose, mesophyll, synchrotron radiation Fourier-transform infrared (SR-FTIR) spectromicroscopy, xylem.

For further information contact Michael Thelen (925) 422-6547 (thelen1@llnl.gov).

Patents and Awards

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Laser Beam Guard Clamps
Richard K. Dickson
U.S. Patent 7,798,459 B2
September 21, 2010
The quick insert and release clamping apparatus for laser beam guard panels has a base plate for mounting on an optical table. One jaw of the apparatus is affixed to the base plate, and a second spring-loaded jaw slides along the base plate to exert a clamping force. Each jaw has a face acutely angled relative to the other face to form a V-shape, open-channel mouth, which enables wedge-action jaw separation by and subsequent clamping of a laser beam guard panel inserted through the open-channel mouth. Preferably, the clamping apparatus also includes a support structure with an open slot aperture positioned over and parallel with the open-channel mouth.

Solid Materials for Removing Arsenic and Method Thereof
Paul R. Coronado, Sabre J. Coleman, Robert D. Sanner, Victoria L. Dias, John G. Reynolds
U.S. Patent 7,803,737 B2
September 28, 2010
Solid materials have been developed to remove arsenic compounds from aqueous media. The arsenic is removed by passing the aqueous stream through the solid materials, which can be in molded, granular, or powder form. The solid materials adsorb the arsenic, leaving a purified aqueous stream. These materials are aerogels or xerogels and aerogels or xerogels and a solid support structure (for example, granulated active carbon mixtures). The species-specific adsorption occurs through chemical modifications of the solids tailored for arsenic.

Optically Pumped Alkali Laser and Amplifier Using Helium-3 Buffer Gas
Raymond J. Beach, Ralph Page, Thomas Soules, Eddy Stappaerts, Sheldon Shao Quan Wu
U.S. Patent 7,804,876 B2
September 28, 2010
In one embodiment, a laser oscillator comprises an optical cavity with a gain medium of an alkali vapor and a buffer gas. The buffer gas includes helium-3 gas, wherein if helium-4 gas is also present in the buffer gas, the ratio of the concentration of the helium-3 gas to the helium-4 gas is greater than 1.37×10^{-6}. An optical excitation source is provided. The laser oscillator is capable of outputting radiation at a first frequency. In another embodiment, an apparatus comprises a gain medium consisting of an alkali vapor and a buffer gas. The buffer gas includes helium-3 gas, wherein if helium-4 gas is also present in the buffer gas, the ratio of the concentration of the helium-3 gas to the helium-4 gas is greater than 1.37×10^{-6}. Other embodiments are also disclosed.

Inspection Tester for Explosives
Jeffrey S. Haas, Randall L. Simpson, Joe H. Satcher
U.S. Patent 7,807,104 B2
October 5, 2010
Nontechnical personnel at any location can use this primary screening tool to determine if a surface contains explosives. First and second explosives-detecting reagent holders and dispensers are connected to the body and positioned to deliver the explosives-detecting reagents to a sample pad. A heater is connected to the sample pad.

Parallel-Aware, Dedicated Job Co-Scheduling within and across Symmetric Multiprocessing Nodes
Terry R. Jones, Pythagoras C. Watson, William Tuel, Larry Brenner, Patrick Caffrey, Jeffrey Fier
U.S. Patent 7,810,093 B2
October 5, 2010
In a parallel computing environment comprising a network of symmetric multiprocessing nodes, with each having at least one processor, a parallel-aware coscheduling method and system improves the performance and scalability of a dedicated parallel job with synchronizing collective operations. The method and system use a global coscheduler and an operating-system kernel dispatcher adapted to coordinate interfering system and daemon activities on a node and across nodes to promote intranode and internode overlap of said interfering system and daemon activities as well as intranode and internode overlap of said synchronizing collective operations. The impact of random short-lived interruptions such as timer-decrement processing and periodic daemon activity on synchronizing collective operations is minimized in large-processor-count SPMD (single process, multiple data) bulk-synchronous programming styles.

System of Fabricating a Flexible Electrode Array
Peter Krulevitch, Dennis L. Polla, Mariam N. Maghribi, Julie Hamilton, S. Humayun, James D. Weiland
U.S. Patent 7,810,233 B2
October 12, 2010
An image is captured or otherwise converted into a signal in an artificial vision system. The signal is transmitted to the retina using an implant. The implant consists of a polymer substrate made of a compliant material such as poly(dimethylsiloxane). The polymer substrate is conformable to the shape of the retina. Electrodes and conductive leads are embedded in the polymer substrate and transmit the signal representing the image to the cells in the retina. The signal representing the image stimulates cells in the retina.

Self-Pressurizing Stirling Engine
Charles L. Bennett
U.S. Patent 7,810,325 B2
October 12, 2010
A solar-thermal-powered aircraft carries a heat engine, such as a Stirling, to produce energy for a propulsion mechanism such as a propeller. The heat engine is connected to a thermal battery. A solar concentrator, such as a reflective parabolic trough, is connected to an optically transparent section of the aircraft body for receiving and concentrating solar energy from within the aircraft. A conduit collects concentrated solar energy and transports it to the thermal battery. A solar tracker includes a heliostat that determines optimal alignment with the Sun and a drive motor that actuates the solar concentrator into optimal alignment with the Sun based on the determination made by the heliostat.

Aerogel and Xerogel Composites for Use as Carbon Anodes

John F. Cooper, Thomas M. Tillotson, Lawrence W. Hrubesh
U.S. Patent 7,811,711 B2
October 12, 2010

With this method, a reinforced rigid anode monolith can be formed to generate fuel for producing electrical energy. The method provides a solution of organic aerogel or xerogel precursors including at least one of a phenolic resin, phenol (hydroxybenzene), resorcinol (1,3-dihydroxybenzene), or catechol (l,2-dihydroxybenzene); at least one aldehyde compound selected from the group consisting of formaldehyde, acetaldehyde, and furfuraldehyde; and an alkali carbonate or phosphoric acid catalyst. Internal reinforcement materials comprising carbon are added to this solution to form a precursor mixture. The mixture is formed into a composite gel and dried. The gel is pyrolyzed to form a wettable aerogel–carbon composite or a wettable xerogel–carbon composite. The composite comprises chars and internal reinforcement materials. It is suitable for use as an anode with the chars providing fuel capable of combustion between 500 and 800°C in a molten salt electrochemical cell to produce electrical energy.

Portable Convertible Blast Effects Shield

John W. Pastrnak, Rocky Hollaway, Carl D. Henning, Steve Deteresa, Walter Grundler, Lisle B. Hagler, Edwin Kokko, Vernon A. Switzer
U.S. Patent 7,819,049 B2
October 26, 2010

A rapidly deployable portable convertible blast effects–ballistic shield includes a set of two or more telescoping cylindrical rings connected to each other to convert between a telescopically collapsed configuration for storage and transport, and a telescopically extended upright configuration forming an expanded inner volume. In one setup, the upright configuration provides blast effects shielding, for example, against blast pressures, shrapnel, or fireballs. In a second setup, the upright configuration provides ballistic shielding against incoming weapons fire and shrapnel. Each ring has a high-strength material construction, such as a composite fiber and matrix material, that can inhibit blast effects and impinging projectiles from passing through the shield. In the telescopically extended upright configuration, the set of rings can be secured to or released from each other by click locks.

Vehicle Underbody Fairing

Jason M. Ortega, Kambiz Salari, Rose McCallen
U.S. Patent 7,828,368 B2
November 9, 2010

This underbody fairing reduces the aerodynamic drag caused by a vehicle wheel assembly. The apparatus reduces the size of the recirculation zone formed under the vehicle downstream of the wheel assembly. A tapered aerodynamic surface extending from the front end to the rear of the fairing body has a U-shaped cross section that tapers in both height and width. Fasteners or other mounting devices secure the fairing body to the underside surface of a vehicle's body, so that the front end is immediately downstream of the wheel assembly. The bottom section of the tapered surface rises toward the vehicle's underside surface as it extends in a downstream direction.

Carbon Ion Pump for Removal of Carbon Dioxide from Combustion Gas and Other Gas Mixtures

Roger D. Aines, William L. Bourcier
U.S. Patent 7,828,883 B2
November 9, 2010

An ion pump method is designed to separate carbon dioxide from flue gas. Current systems rely on large changes in temperature or pressure to remove carbon dioxide from a solvent used to absorb it from flue gas. In contrast, the ion pump method increases the concentration of dissolved carbonate ion in solution, which increases the overlying vapor pressure of carbon dioxide gas. As a result, carbon dioxide can be removed as a pure gas on the downstream side of the pump. Ion pumping may be obtained from reverse osmosis, electrodialysis, or thermal desalination or from an ion pump system with an oscillating flow synchronized with an induced electric field.

Simple, Field Portable Colorimetric Detection Device for Organic Peroxides and Hydrogen Peroxide

Philip F. Pagoria, Alexander R. Mitchell, Richard E. Whipple, M. Leslie Carman, John G. Reynolds, Peter Nunes, Sharon J. Shields
U.S. Patent 7,829,020 B2
November 9, 2010

This simple system uses changes in a reagent's color to quickly determine if organic peroxides or hydrogen peroxide is present. A peroxide pen has a swipe material attached to a polyethylene tube and two crushable vials. The vials contain a colorimetric reagent separated into dry and liquid ingredients. Once the pen is swiped across a suspected substance or surface, the vials are broken, and the reagent is mixed thoroughly. It is then allowed to wick into the swipe material. The presence of organic peroxides or hydrogen peroxide is confirmed if the reagent turns deep blue.

Grating Enhanced Solid-State Laser Amplifiers

Alvin C. Erlandson, Jerald A. Britten
U.S. Patent 7,830,946 B2
November 9, 2010

This apparatus suppresses amplified spontaneous emission (ASE) and parasitic oscillation modes in a high-average-power laser. The system uses diffraction gratings to increase the gain, stored energy density, and pumping efficiency of a solid-state laser gain media, such as rods, disks, and slabs. ASE and parasitic oscillation modes can be effectively suppressed by coupling predetermined gratings to the solid-state gain media used in crystal or ceramic lasers.

Awards

Kim Budil, a Laboratory employee on assignment in Washington, DC, to the **National Nuclear Security Administration** (NNSA), received a rarely bestowed honor, the NNSA **Administrator's Award for Excellence Medal**, for distinguished service in the national security interests of the U.S. Budil had been working within the Weapons and Complex Integration Principal Directorate, when she was selected a year and a half ago by the Department of Energy's Undersecretary for Science, Steve Koonin, to serve as a senior adviser on science related to national security. Among her assignments was developing an agenda and organizing a two-day senior review with external experts about the nuclear weapons stockpile and the technical skills needed to sustain it. Budil's other activities included organizing a review by the National Academy of Sciences on inertial fusion energy and Koonin's review of the National Ignition Campaign.

In November 2010, at the R&D 100 Awards ceremony sponsored by ***R&D Magazine***, a Livermore team and its partners received an **Editors' Award**, signifying the utmost achievement in developing new technology. This year, the honor went to **Hyung Gyu Park** and **Francesco Fornasiero**, for their work developing nanostructured membranes for water purification. The technology has been licensed to Porifera, Inc., of Hayward, California. Livermore also received six R&D 100 awards in the annual competition for the top 100 industrial, high-technology inventions. (See *S&TR*, October/November 2010, pp. 4–15.)

John Elmer, a scientist in Livermore's Physical and Life Sciences Directorate, received the **McKay–Helm Award** from the **American Welding Society** for his paper, "Heat Transfer and Fluid Flow during Electron Beam Welding of 304L Stainless Steel Alloy," which was published in the March 2009 issue of *Welding Journal*. The McKay–Helm Award honors the best contribution to the advancement of knowledge of low-alloy steel, stainless steel, or surfacing welding metals involving the use, development, or testing of these materials, as represented by articles published in *Welding Journal* during the previous calendar year. Elmer is a fellow of the American Welding Society and has received several awards from the organization.

Abstract

Groundbreaking Science with the World's Brightest X Rays

Livermore researchers are conducting experiments at the Linac Coherent Light Source (LCLS), which produces ultrafast x-ray pulses more than a billion times brighter than ever produced on Earth. Located at the Department of Energy's SLAC National Accelerator Laboratory in Menlo Park, California, LCLS was designed to enable scientists to take stop-action pictures of atoms and molecules in motion. Livermore experts designed and fabricated the optics that transport the x-ray beam to chambers in two experimental halls. These mirrors help control the size and direction of the x-ray beam. Additional detectors fabricated by Livermore help diagnose x-ray beam properties such as intensity. LCLS is the world's most powerful x-ray free-electron laser. Its photons are coherent, meaning they act in unison, and thus are well suited for imaging applications. LCLS pulses are of extremely short duration, lasting between 10 and 100 femtoseconds, and the photons have wavelengths about 10 times shorter than can be produced by other x-ray free-electron lasers. Although the powerful beam destroys each sample, the ultrashort pulse generates diffraction data before that occurs. By sequencing separate stop-action images taken with LCLS pulses, scientists will also be able to create time-resolved movies, permitting them to view the formation and breaking of chemical bonds in real time.

Contact: Stefan Hau-Riege (925) 422-5892 (hauriege1@llnl.gov).

U.S. Government Printing Office: 2011/770-075-50002

A Natural Enzyme for Carbon Capture

A molecule that mimics the way our lungs and blood separate carbon dioxide may help coal-fired power plants capture this greenhouse gas.

Also in March

• Livermore experts took part in an international collaboration to stop the undersea oil spill in the Gulf of Mexico.

• An innovative adaptive modeling framework analyzes the often difficult-to-trace steps taken in adversarial transactions.

• A new open campus at Lawrence Livermore and Sandia national laboratories aims to strengthen partnerships with industry and universities.

Coming Next Issue

Science & Technology Review
Lawrence Livermore National Laboratory
P.O. Box 808, L-664
Livermore, California 94551

PRSRT STD
U.S. POSTAGE
PAID
San Bernardino, CA
PERMIT NO. 3330

Printed on recycled paper.